Effect of antisite-like defect in ferroelectricity of SrTiO₃ films

FANG YANG, ZHENZHONG YANG, LIN GU, JIANDONG GUO, Institute of Physics, Chinese Academy of Sciences, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM — Ferroelectricity in thin films of nominally nonferroelectric materials such as SrTiO₃ has been widely studied. It is known that some extrinsic factors such as strain [M. P. Warusawithana et al. Science 324, 367 (2009)] and defect [H. W. Jang et al., Phys. Rev. Lett. 104, 197601 (2010), M. Choi et al., Phys. Rev. Lett. 103, 185502 (2009)] can result in the ferroelectricity of SrTiO₃ thin films. The SrTiO₃ thin films with ferroelectricity were prepared on Si (001) substrates by oxide molecular beam epitaxy. The energy dispersive x-ray spectroscopy (EDX) mapping measurement results demonstrate Sr diffuses to the interface of SrTiO₃ and Si. The cross sectional high-resolution transmission electron microscopy (HRTEM) results show that there are interstitial Ti atoms in the unit cells. The off-centered Ti from the Sr site along [100] or [110] direction can be regarded as a polar defect pair composed of a Sr vacancy and an interstitial Ti. It is predicted that Ti antisite-like defects in SrTiO₃ are responsible for the ferroelectricity. Such antisite-like defects observed in SrTiO₃ films are considered as the origin of the ferroelectricity.

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